

Hydrogenic Spin Quantum Computing in Silicon: a Digital Approach

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(Dated: January 29, 2003)

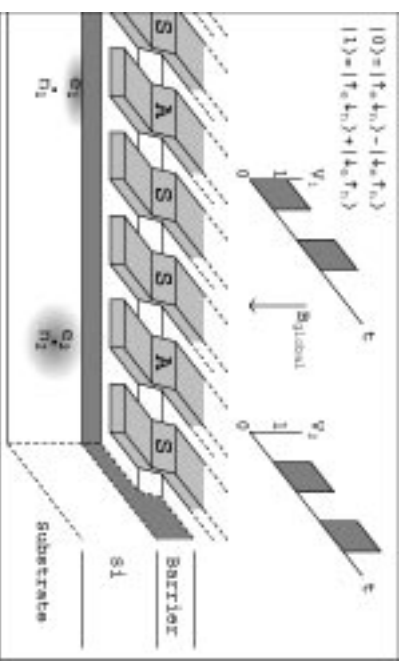
We suggest an architecture for quantum computing with spin-pair encoded qubits in silicon. Electron-nuclear spin-pairs are controlled by a DC magnetic field and electrode-switched on and off hyperfine interaction. This digital processing is insensitive to tuning errors and easy to model. Electron shuttling between donors enables multi-qubit logic. These hydrogenic spin qubits are transferable to nuclear spin-pairs, which have long coherence times, and electron spin-pairs, which are ideally suited for measurement and initialization. The architecture is scalable to highly parallel operation.

PACS numbers: 03.67.Lx, 72.25.Dc

Donor nuclear spins are good qubits for silicon-based quantum computing and can in principle be controlled by hyperfine-tuned magnetic resonance techniques and coupled by the electron exchange interaction [1]. However, this “exchange mediation” in Si is extremely difficult to control [2, 3] and exhibits oscillatory behavior [4, 5]. Precise tuning of the hyperfine interaction will also be difficult. Error-correction schemes [6] and decoherence-free subspaces [7, 8, 9, 10, 11] suggest encoding each logical qubit in multiple spins. Indeed, encoding can result in reduced constraints on computer design [12]. In the context of spin based computing, DiVincenzo et al. developed techniques for exchange-only control of qubits encoded in three electron spins [3, 14, 15]. By including a static magnetic field, Levy proposed Heisenberg-only quantum computing for qubits encoded in the $J_z = 0$ subspace of two spins with different magnetic moments [12, 16, 17].

These ideas are naturally applied to hydrogenic spin qubits, in which electron and donor nuclear spins have distinct magnetic moments and are coupled by the hyperfine interaction tuned by the electron’s charge configuration. The ground state coupling for P donors in Si, $H_A = A\vec{\sigma}_e \cdot \vec{\sigma}_n$, is ideally suited to quantum computing because it is well known ($\vec{\sigma} \equiv (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli operators, labelled by the spin on which they operate; $A = 121.517 \pm 0.021$ neV [18]) and stable; its strength is determined by the electron-donor overlap, $|\psi(0)|^2$, which is a quadratic function of small perturbations in electric field strength. When the electron is drawn away from the nucleus to an interface state (see Figure 1), the ionized coupling, $H_A = 0$, is similarly stable. These two extremes are insensitive to tuning errors and we therefore adopt a binary approach, in which the interaction is only on or off for sufficient time to give the desired integrated strength.

Our error analyses of canonical one- and two-qubit logic gates, simulated with explicit digital control sequences, show that efficient quantum computation is possible with the following architecture. Each qubit is en-



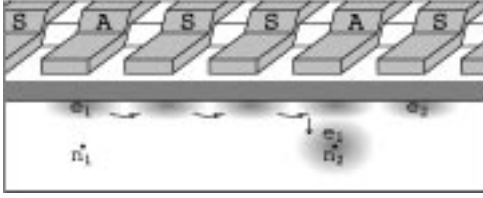


FIG. 2: Entangling qubits e_1n_1 and e_2n_2 . S-gates displace e_2 and shuttle e_1 to the vicinity of n_2 . The A-gate above n_2 then applies hyperfine interaction, generating a partial e_1 - n_2 spin swap.

been demonstrated [19], so single electron shuttling [20] to remote donor sites is a good candidate for enabling two-qubit interaction. This is analogous to ion-trap proposals in which ions, and thus their quantum information, can be shuttled from one local trap to another [21, 22]. As shown in Figure 2, arrays of “S-gate” electrodes between qubits are thus used to shuttle individual electrons from site to site. Two qubits become entangled when the hyperfine interaction is applied between the electron of one qubit and the nucleus of another.

The evolution of the electron and donor spins is described by their Hamiltonian,

$$H = \sum_{i,j} A_{ij} \vec{\sigma}_{e_i} \cdot \vec{\sigma}_{n_j} + \sum_i B (g_e \mu_B \sigma_{e_i}^z - g_n \mu_N \sigma_{n_i}^z).$$

The second term, H_B , sums the contribution from all donors and their electrons, with respective magnetic moments $g_n \mu_N$ and $g_e \mu_B$, in the vertical magnetic field B assumed parallel to a (100) lattice plane. It augments the hyperfine contact term, H_A , which is a sum of interactions between electron-donor pairs. Interaction between the i th electron and the j th donor is either off ($A_{ij} = 0$) or on ($A_{ij} = A$). We assume instantaneous switching and neglect the spin-orbit and dipole-dipole interactions (which are zero for the ground state and for sufficiently large r but finite in-between) as well as any randomness in the contact strength during the switch. For P donors in Si the ground and first excited orbitals are separated by ≈ 5 meV; a more realistic adiabatic switch takes $\mathcal{O}(10)$ ps which is fast compared to the hyperfine interaction.

The state space of spins is decomposable into invariant subspaces labelled by the z component of the total spin; up and down spins are stationary states of H_B while electron-donor spin swaps, generated by H_A , preserve the number of up vs. down spins. Within each invariant subspace flipping an electron spin, which changes the energy by $\Delta E_e = 2Bg_e\mu_B$ has a compensatory nuclear spin flip, which changes the energy by a further $\Delta E_n = 2Bg_n\mu_N$, and the magnetic energy splittings are thus integer multiples of $\Delta E_r = \Delta E_e + \Delta E_n$. Transitions between subspaces require the flipping of one spin or the other and thus there are non-resonant shifts ΔE_e and ΔE_n between

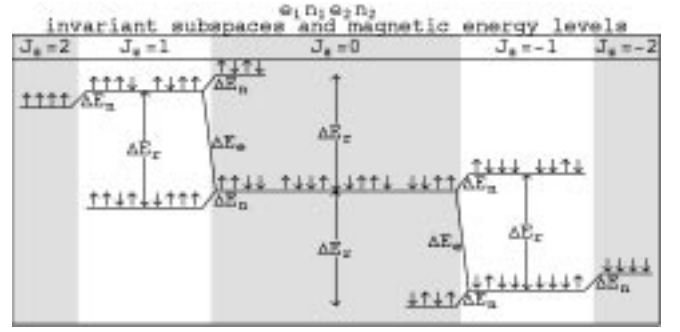


FIG. 3: Magnetic energy levels and invariant subspaces of a two-qubit computer. Flipping a single electron or single nuclear spin changes the energy by ΔE_e or ΔE_n respectively and takes the state to another subspace. Within an invariant subspace, simultaneous electron and donor spin flips change the energy by $\Delta E_r = \Delta E_e + \Delta E_n$.

subspaces. As a specific example Figure 3 shows the magnetic energy levels and invariant subspaces of a two-qubit computer.

It is desirable to generate pure hyperfine evolution even though the magnetic field is, in fact, always present. We make use of the Trotter formula [6],

$$e^{-iH_A t/\hbar} \approx (e^{iH_B \Delta t/2\hbar} e^{-i(H_A + H_B) \Delta t/\hbar} e^{iH_B \Delta t/2\hbar})^a,$$

and compose a finite duration, t , of hyperfine evolution with a large number, a , of short $\Delta t = t/a$ steps of hyperfine *and* magnetic evolution corrected, on the fly, by time-reversed $\Delta t/2$ steps of solely magnetic interaction. Although magnetic and hyperfine steps do not commute, the remaining error of each step after correction, by a variant of the Campbell-Baker-Hausdorff formula [6], is $\mathcal{O}(\Delta t^3)$ and increases with magnetic field (the non-commutativity, $[H_A, H_B]$, scales with B); we can achieve good fidelity with sufficiently short Δt steps and a sufficiently weak field.

Within each invariant subspace the time-reversed magnetic steps are achieved by incomplete periods of magnetic evolution. A full period is determined by the energy splitting: $T_B = \hbar/\Delta E_r$ (see Figure 3). We need only wait $T_B - \Delta t/2$ to achieve the magnetic correction step. In analogy with magnetic resonance techniques we thus proceed by resonant stepping; for each period of magnetic evolution there is a short step of $H_A + H_B$. The result is true hyperfine evolution up to relative phase shifts between invariant subspaces.

The use of digital bit trains from a pulse pattern generator considerably simplifies the timing of these operations. For example, we divide the fixed hyperfine period, $T_A = \hbar/4A = 8.50847$ ns, into 96 clock cycles by setting the frequency at $f = 11.2829$ GHz; given this frequency we then divide the magnetic period T_B into 256 clock cycles by choosing a field strength of $B = 1.57171$ mT.

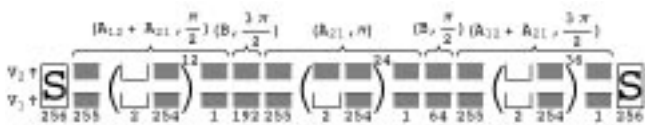


FIG. 4: Operations timeline for an entangler. The diagram depicts a sequence of on-or-off A-gate voltages and their duration in clock cycles. Hyperfine interaction is on whenever the voltage is off. The magnetic field is always on. The shuttling of electrons is represented schematically but would be effected by a sequence of S-gate voltage pulses.

Within an invariant subspace, generating pure hyperfine evolution is now as simple as turning off certain A-gate voltages for 2 clock cycles out of every 256.

The encoded qubits reside in the $J_z = 0$ invariant subspace. We can thus construct logic operations from finite ϕ pulses of magnetic evolution, $(B, \phi) \equiv e^{-iH_B \phi T_B / \hbar}$, and θ pulses of pure hyperfine evolution, $(A, \theta) \equiv e^{-iH_A \theta T_A / \hbar}$, implemented with resonant hyperfine stepping. The Controlled-Not (CNOT) operation, which performs a logical NOT operation on a second qubit contingent on the state of a first, can, for example, be implemented in the following manner:

$$CNOT = (L_1 \otimes Z_2) N (L_1 \otimes Z_2)^\dagger,$$

in which single qubit operations,

$$(L_1 \otimes Z_2) = (B, \frac{3\pi}{2})(A_{11} + A_{22}, \pi)(A_{11}, \frac{\pi}{2})(B, \frac{\pi}{2}),$$

augment an entangler,

$$N = (A_{12} + A_{21}, \frac{3\pi}{2})(B, \frac{\pi}{2})(A_{21}, \pi)(B, \frac{3\pi}{2})(A_{12} + A_{21}, \frac{\pi}{2}).$$

This construction refines Levy's original [16] but may not be optimal. Figure 4 depicts the actual sequence of A-gate voltages that implements the entangler, N.

Shorter hyperfine steps and a weaker magnetic field reduce the errors. However, commercially available pulse pattern generators are limited to approximately 12 GHz (hence our choice of $f = 11.2829$ GHz). Furthermore, the preponderance of magnetic periods (one for each small hyperfine step) means that a computation slows with weaker field. There is thus a trade-off between fidelity and speed. Our choice of $B = 1.57171$ mT yields a complete spin-swap (the architecture's fundamental process) in $0.57 \mu\text{s}$. When ideally implemented with resonant hyperfine stepping, its expected error (defined to be the average probability of incorrectly transforming an initial, arbitrary, two-qubit basis of states) is less than 2.1×10^{-7} . The CNOT is our most complicated gate and can be ideally implemented with an expected error of at most 0.9×10^{-6} in $3.22 \mu\text{s}$.

It is unrealistic to presume exact values for the frequency, field, and hyperfine strength. There may also

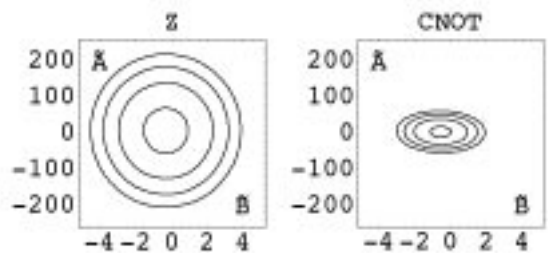


FIG. 5: Simulations of Z and CNOT logic gates produced $(0.1, 0.4, 0.7, \& 1.0) \times 10^{-5}$ error ellipses showing tolerable variations in magnetic field, $\Delta B/B \equiv 10^{-5} \tilde{B}$, and hyperfine strength, $\Delta A/A \equiv 10^{-5} \tilde{A}$.

be variations of hyperfine and/or field strength from one donor site to the next. Indeed, although isotope purification can remove most Si^{29} from the crystal, the remaining impurities cause field variations (although these fluctuate so slowly that spin-echo techniques may be applicable). Another complication is that the Landé factor for the electron, g_e , will vary slightly between the donor and the Si-Barrier interface [18].

The threshold theorem [6] for quantum computation concludes that efficient quantum computing, obtained with error correction techniques, is possible when logic gate errors are less than 10^{-5} . We have calculated the tolerable variations for canonical one- and two-qubit logic gates. The relative errors in frequency and field can be as large as 10^{-5} while the relative hyperfine error can be 10^{-4} to 10^{-3} . The sensitivity to local variations in these parameters is the same order of magnitude. The fidelity is comparatively insensitive to the hyperfine errors because our gate compositions are predominantly magnetic. Finally, the architecture can tolerate 10^{-3} to 10^{-2} variations in g_e between the donor and the interface. As an example of these error analyses, Figure 5 shows error ellipses for the spin swap ("Z" gate) and the CNOT.

A π pulse of hyperfine interaction, (A, π) , between two qubits generates a complete spin swap between the electron of one qubit and the donor of the other. Considered as a switch to a new encoding scheme, this hyperfine "data bus" transfers one qubit into a nuclear spin-pair and the other into an electron spin-pair. For example, an $e n$ data qubit, with the use of an $e_A n_A$ "ancilla," can be transferred, by resonant hyperfine stepping, into an $n_A n$ nuclear spin-pair qubit. Retrieval simply requires another π pulse to repeat the spin swap.

The relatively weak nuclear magnetic moment gives the nuclear spin a long decoherence time which makes the nuclear spin-pair qubit a natural quantum memory. Furthermore, if the data and ancilla were initially unentangled they remain unentangled, so decoherence or collapse of the ancilla (now encoded in the electron spin-pair) will not degrade the memory (the qubit's transfer succeeds

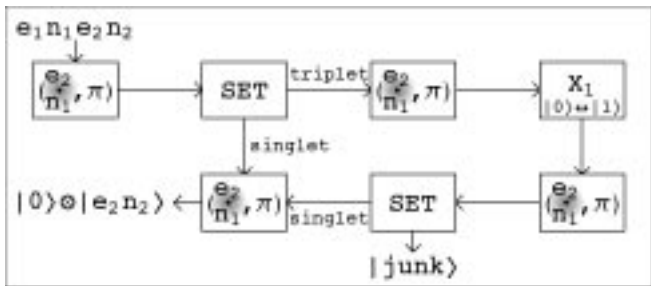


FIG. 6: Qubit Initialization and Sorting. A singlet outcome is immediately convertible into $|0\rangle$ while the triplet outcome can be recycled through a sequence of operations into another chance for a useful singlet.

even when the ancilla is outside its logical subspace; relative phases developed between invariant subspaces, by resonant hyperfine stepping, are absorbed solely into the ancilla).

The data qubit can, alternatively, be transferred into an electron spin-pair to facilitate measurement by various proposed methods to distinguish singlets and triplets. For an electron spin-pair known to reside in the logical subspace, these are effectively $|0\rangle = |\text{singlet}\rangle$ vs. $|1\rangle = |\text{triplet}, S_z = 0\rangle$ projective qubit measurements. For example, a Single Electron Transistor (SET) is capable of very sensitive charge configuration measurements; above a donor it can detect electrode driven charge density fluctuations associated with the electron spin-pair singlet [23]. Alternatively, in a quantum dot the electrons' spin determines the tunneling of spin-polarized currents [24].

After measurement the collapsed electron spin-pair can be transferred back into an electron-donor pair via another spin swap. This provides a way to initialize the computer at high temperature (e. g. 1 K). Read-out collapses an electron spin-pair into a singlet or triplet. The singlet outcome, $|\uparrow_{e1}\downarrow_{e2}\rangle - |\downarrow_{e1}\uparrow_{e2}\rangle$, is immediately convertible, via a spin swap, to $|0\rangle$. The triplet outcome, $|\uparrow_{e1}\uparrow_{e2}\rangle, |\uparrow_{e1}\downarrow_{e2}\rangle + |\downarrow_{e1}\uparrow_{e2}\rangle, \text{ or } |\downarrow_{e1}\downarrow_{e2}\rangle$, can be recycled, as depicted in Figure 6, through a single qubit $|0\rangle \leftrightarrow |1\rangle$ operation sandwiched between spin swaps, for another chance to obtain a useful singlet. (This cascaded measurement prevails despite relative phases developed between invariant subspaces.) At high temperature 50% of the electron-donor pairs will obtain $|0\rangle$, and by electron shuttling the successful 50% can be “pooled” into the working part of the computer in analogy with Kane’s original proposal for on-chip spin refrigeration [25].

Hydrogenic spin qubits and coherent single electron shuttling enable a silicon-based quantum computer featuring digital hyperfine control insensitive to tuning errors, a long-lived nuclear spin memory, a projective read-out scheme, and qubit refrigeration in which 50% of the qubits can be initialized at high temperature.

The computer is scalable to highly parallel operation because digital shuttling of electrons overcomes nearest neighbor restrictions. Finally, donors can be irregularly spaced and far apart, allowing for large gate electrodes, and malfunctioning donor sites can be diagnosed and avoided. These many benefits motivate further research on the coherent shuttling and measurement of electron spins, extremely pure Si fabrication, encoding and error-correction techniques, and the spin-orbit and dipole-dipole interactions during realistic electrode driven switching.

We are grateful for helpful discussions with S. Lomonaco. Research by AJS was done in partial fulfillment of the requirements for the Ph.D. Degree in Physics at the University of Maryland, College Park.

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